Chemical Selection Planning

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Presentation to Scientific Guidance Panel
Oakland, CA
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Purpose of Agenda Item

1. Preliminary screen for possible future consideration as potential designated chemicals

   Some bisphenol A (BPA) substitutes and structurally related compounds

2. Options for revising listing of polycyclic aromatic hydrocarbons (PAHs)

Why screen BPA substitutes and related compounds?

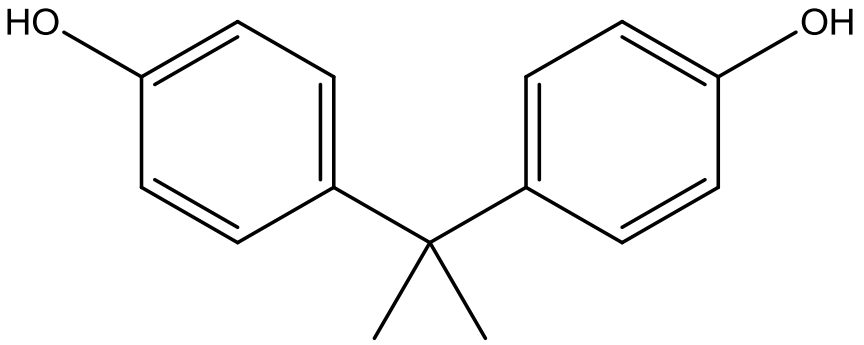
- Public and Panel interest
- Emerging alternatives for BPA, likely to increase in use
- Use in consumer products
- Indications of toxicity

Preliminary screen

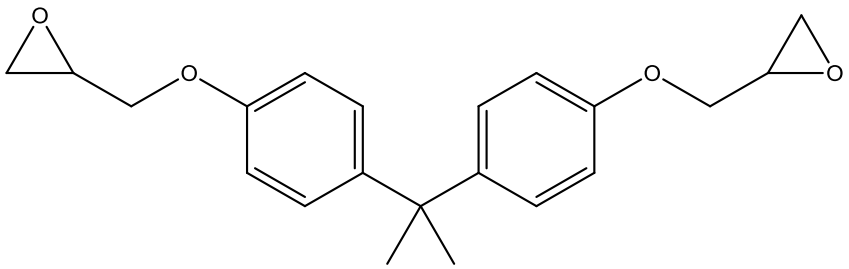
Brief summary of information located so far on 23 substances:

- Chemical identity and structure
- Use and production
- Detection in products or biological or environmental samples
- Physical and chemical properties
- Predicted bioaccumulation and persistence
- Approximate extent of toxicity data and types of endpoints

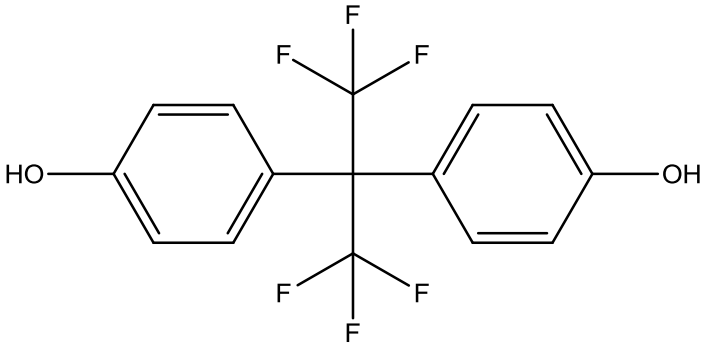
Bisphenol A (BPA)



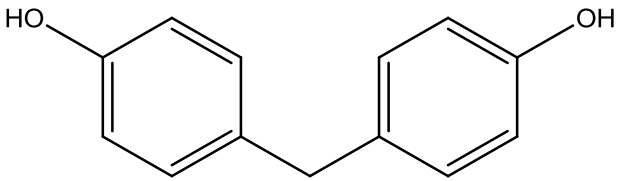
Bisphenol A diglycidyl ether



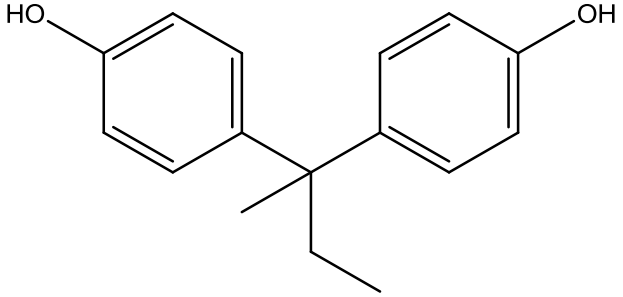
Bisphenol AF



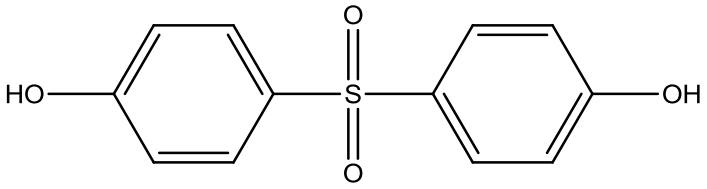
Bisphenol F



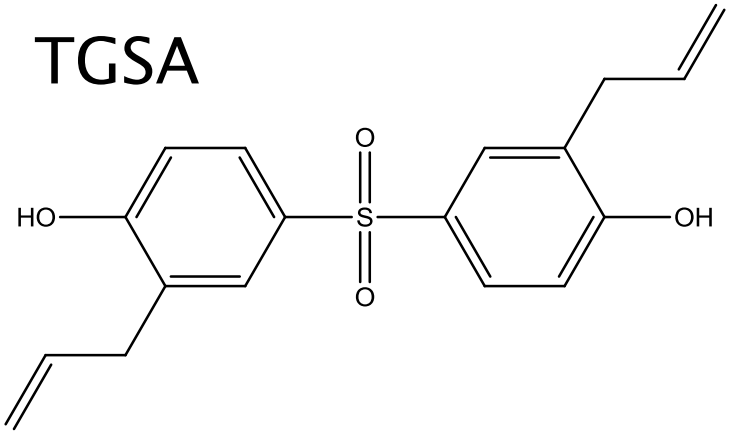
Bisphenol B



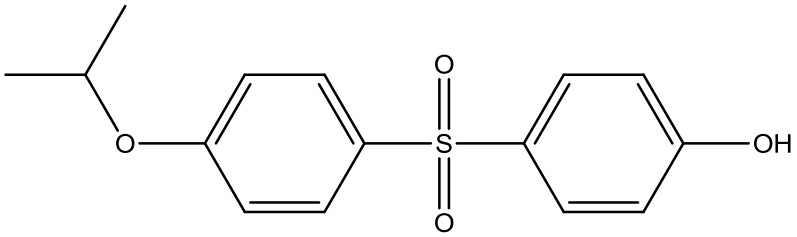
Bisphenol S (BPS)



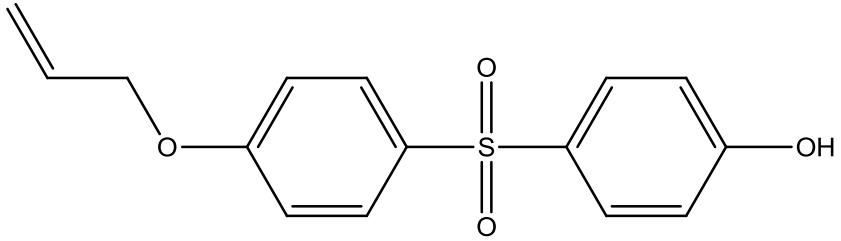
TGSA



D-8

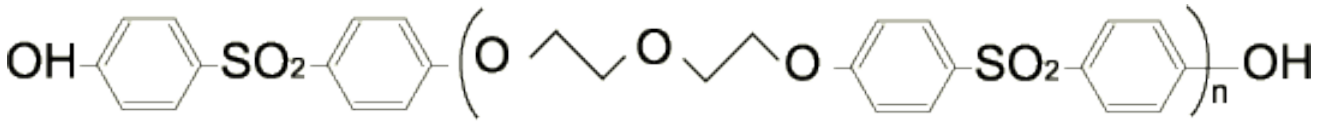


Bisphenol S-MAE

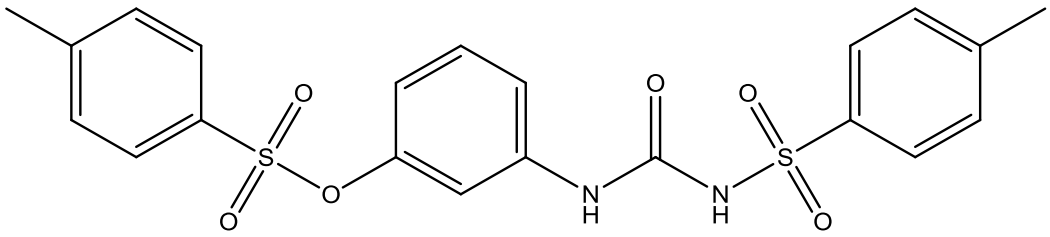


Others related to BPS

D-90

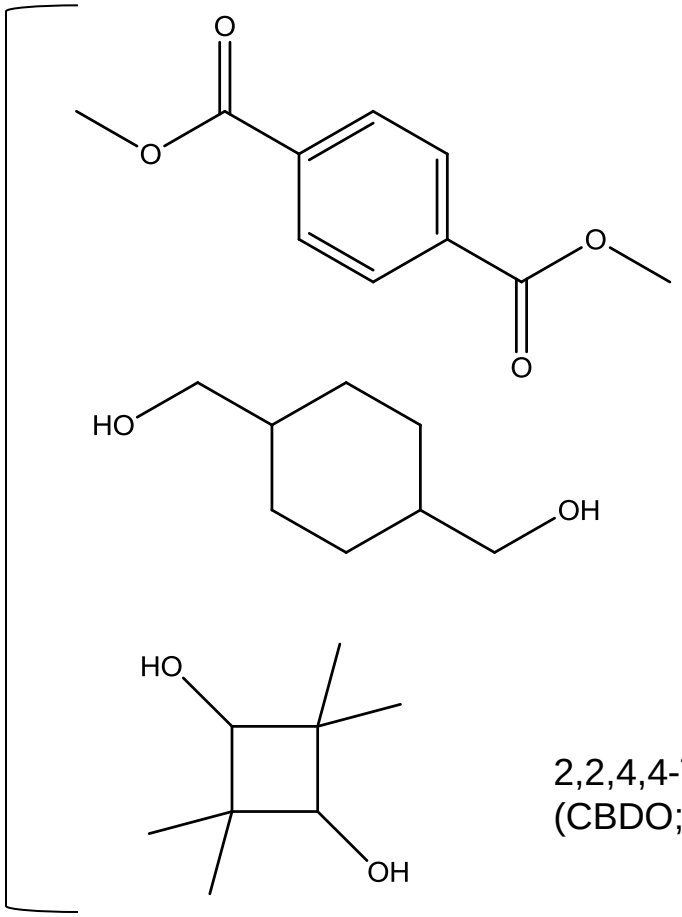


Pergafast 201



Other alternatives

Tritan™ copolymer:



Dimethyl terephthalate (DMTP)

1,4-Cyclohexanedimethanol (CHDM)

2,2,4,4-Tetramethyl-1,3-cyclobutanediol (CBDO; TMCD)

EcoCare™ - Proprietary formulation

Major types of uses

- Protective coatings
  - For example, inside food and beverage containers
- Production of plastics
- Developers in thermal paper
  - For example, in cash register receipts

Production/Import Volume (2006)

Volume (lbs)	Chemicals
> 1 B	• BPA (*for comparison*) • DMTP (Tritan™ monomer)
100 – < 500 M	• CDHM (Tritan™ monomer)
1– <10 M	• BADGE • BPS (4,4'–) • TGSA • D–8
<500 K	• BPAF • BPS (2,4'–) • CBDO (Tritan™ monomer)
No Production Volume Located	• BPAP • BPB • BPC • BPF • BFDGE • PHBB • MBHA • BisOPP–A • 1,7–Bis…heptane • BPS–MAE • BPS–MPE • D–90 • Pergafast 201 • Urea urethane compound • BTUM • EcoCare™

Source: *US EPA, Toxic Substances Control Act (TSCA) Inventory Update Reporting for 2006*

Predicted bioaccumulation & environmental persistence (selected results)

Chemical name	BCF	Half-lives (days)		
		Water	Soil	Marine sediment
BPA	**72**	**38**	**75**	**340**
BADGE	160	**60**	**120**	**540**
BPAF	420	**180**	**360**	**1600**
BisOPP-A	**11,000**	38	**75**	**340**
4,4'-BPS	5.7	15	30	**140**
TGSA	390	38	**75**	**340**
D-8	53	38	**75**	**340**
BPS-MPE	180	38	**75**	**340**
D-90 (example compound)	150	**60**	**120**	**540**
Pergafast 201	280	**60**	**120**	**540**
Urea urethane compound (example compound)	**9100**	**180**	**360**	**1600**
BTUM	370	**60**	**120**	**540**

Notes*: Predictions generated with PBT Profiler. **Orange** indicates persistent; **red** indicates very bioaccumulative or very persistent (based on US EPA criteria).*

Toxicity – preliminary screen

- Many have limited or no toxicity data
- Literature studies found so far include:
  - *In vivo* – uterotrophic assay
  - *In vitro* – assays for endocrine disrupting activity; genotoxicity

Toxicity – preliminary screen (cont).

Chemical name	Evidence of endocrine disrupting activity - *in vitro assays*	Evidence of estrogenicity - *uterotrophic assay*
BADGE	X	
BPAF	X	X
BPAP	X	
BPB	X	X
BPF	X	X
BFDGE	X	
PHBB	X	
4,4'-BPS	X	X
D-8	X	

US EPA's Design for the Environment

- US EPA's DfE conducting assessment of functional alternatives for BPA in thermal paper, based on:
  - Human and environmental health profiles
  - Structure-activity modeling
  - Proprietary information
- Draft report due out in late March, early April

Questions for the Panel

What next steps should the Program take for BPA substitutes and structurally related compounds?

Options include –

- Additional screening:
  - Laboratory research: Investigate possible pilot screening of urine and/or blood samples from volunteers
  - Library research: Expand preliminary screen

- Potential designated document(s) on:
  - A sub-set (e.g., defined by chemical structure and/or use)
  - Selected individual chemicals

Revising listing of PAHs as designated and priority chemicals

Background

- Designated PAHs based on CDC
- Priority PAHs
  - In 2009, the Panel recommended 3 hydroxy-PAHs as priority chemicals based on predicted lab capability
- Lab now has capability for many more

Revising listing of PAHs as designated and priority chemicals

Proposal

- Program develops one-pager to support Panel consideration of PAHs as a class for designation
- Panel could later consider recommending the full class of PAHs, or a sub-set of PAHs, as priority chemicals